

Theory of magnetic excitons in the heavy-fermion superconductor UPd₂Al₃

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We analyze the influence of unconventional superconductivity on the magnetic excitations in the heavy fermion compound UPd₂Al₃. We show that it leads to the formation of a bound state at energies well below $2\Delta_0$ at the antiferromagnetic wave vector $\mathbf{Q}=(0,0,\pi/c)$. Its signature is a resonance peak in the spectrum of magnetic excitations in good agreement with results from inelastic neutron scattering. Furthermore we investigate the influence of antiferromagnetic order on the formation of the resonance peak. We find that its intensity is enhanced due to intraband transitions induced by the reconstruction of Fermi surface sheets. We determine the dispersion of the resonance peak near \mathbf{Q} and show that it is dominated by the magnetic exciton dispersion associated with local moments. We demonstrate by a microscopic calculation that UPd₂Al₃ is another example in which the unconventional nature of the superconducting order parameter can be probed by means of inelastic neutron scattering and determined unambiguously.

I. INTRODUCTION

The relationship between unconventional superconductivity and magnetism in heavy-fermion systems and transition metal oxides is one of the most interesting research areas in condensed matter physics. In both cases it is widely believed that the magnetic degrees of freedom play an essential role in the formation of superconductivity. Furthermore, unconventional superconductivity yields strong feedback on the magnetic spin excitations in these systems below the superconducting transition temperature T_c . One example is the famous so-called resonance peak observed in high- T_c cuprates by means of inelastic neutron scattering (INS)¹ whose nature is still actively debated.² Remarkably, it has been found that INS reveals the formation of a new magnetic mode in the superconducting state of the uranium based heavy-fermion compound UPd₂Al₃ with $T_c = 1.8$ K.³ Its sharply peaked intensity, its temperature dependence and the energy position well below $2\Delta_0$ (with Δ_0 being the maximum of the superconducting gap) strongly resembles the resonance peak seen in high- T_c cuprates. This is particularly remarkable, since the origin of superconductivity in cuprates and UPd₂Al₃ seems to be different. While frequently discussed scenarios in cuprates are a spin-fluctuation mediated Cooper pairing or the electron-phonon interaction, in UPd₂Al₃ a magnetic-exciton mediated pairing model has been proposed⁵ based on available experiments. The latter model is built on the dual nature of the $5f$ electrons. It consists of localized $5f^2$ crystalline electric field (CEF) states which disperse into a magnetic exciton band due to intersite interactions and a conduction electron band⁴ formed by itinerant $5f$ electrons with enhanced hybridization. The model successfully explains the formation of unconventional superconductivity in this compound⁵ based on the virtual exchange of the magnetic excitons between itinerant quasiparticles.

It is important to note that the resonant spin excitations in superconducting cuprates can be seen as a direct consequence of the $d_{x^2-y^2}$ -wave symmetry of the superconducting order parameter. Namely, the resonance peak occurs only if the order parameter changes sign in the first Brillouin zone (BZ).⁶ Thus, INS can be considered as a bulk probe for the unconventional nature of superconductivity in these compounds. Therefore it is important to search for such an effect in other unconventional superconductors as well. In this paper we analyze the consequences of the unconventional pairing on the magnetic excitations in UPd₂Al₃. We show that in addition to the magnetic exciton dispersion present in the normal state, unconventional superconductivity induces the formation of a bound state below T_c with an associated resonance peak in the magnetic spectrum at the antiferromagnetic (AF) wave vector $\mathbf{Q}=(0,0,\pi/c)$ where c is a lattice constant along the crystallographic z axis. Its frequency is well below $2\Delta_0$ and in good agreement with experimental data. We show that similar to cuprates the resonance peak in UPd₂Al₃ is a consequence of an unconventional superconducting order parameter which changes sign at regions of the Fermi surface connected by the antiferromagnetic wave vector \mathbf{Q} . We analyze the influence of antiferromagnetism on the formation of the resonance peak and surprisingly find that its intensity is enhanced due to the reconstruction of the Fermi surface. We find that the dispersion of the resonance peak away from \mathbf{Q} is controlled by the momentum dependence of excitations of the localized magnetic moment (magnetic exciton).

The resonance peak in UPd₂Al₃ has also been studied by Bernhoeft et al.⁷ within a phenomenological two component spin susceptibility model. However, in our microscopic calculations we show that antiferromagnetic order plays a crucial role in the formation of the resonance peak below T_c .

II. THE HAMILTONIAN

Following previous consideration by McHale *et al.*⁵ we use the low-energy Hamiltonian describing the interaction of the itinerant f electrons and magnetic excitons originating from localized $5f^2$ crystalline electric field (CEF) states:

$$H_0 = \sum_{\mathbf{p}\sigma} \xi_{\mathbf{p}} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \left(\alpha_{\mathbf{q}}^\dagger \alpha_{\mathbf{q}} + \frac{1}{2} \right) - \frac{g}{N} \sum_{\mathbf{p}, \mathbf{q}} c_{\mathbf{p}\alpha}^\dagger \sigma_{\alpha\beta}^z c_{\mathbf{p}+\mathbf{q}, \beta} \lambda_{\mathbf{q}} \left(\alpha_{\mathbf{q}} + \alpha_{-\mathbf{q}}^\dagger \right), \quad (1)$$

where $\lambda_{\mathbf{q}}^2 = \frac{\Delta_{\text{CEF}}}{\omega_{\mathbf{q}}}$, and $\Delta_{\text{CEF}} = 6$ meV is the energy gap of the $5f^2$ electrons between the ground and first excited states in the crystalline electric field. The dispersion of the magnetic excitons is approximately described by $\omega(q_z) = \omega_{ex}[1 + \beta \cos(q_z)]$ with $0 < \beta \simeq 1$, where g is the coupling constant between the itinerant electrons and the localized magnetic moments. We adopt parameter values $\omega_{ex} = 5.5$ meV and $\beta = 0.72$. Note, here we follow Ref. 5 in assuming that only the σ_z component of the conduction electrons can excite magnetic excitons. Therefore the spin-space isotropy is broken in a maximal (Ising) way. As a result the usual classification of Cooper pairs into spin-triplet and spin-singlet states is not valid and the notation equal and opposite spin pairing states should be better used instead. However, we will still speak of singlet and triplet Cooper-pairing states as

commonly done.

Eq. (1) gives rise to fermionic and bosonic self-energies and is particularly relevant for electron-hole states separated by the antiferromagnetic wave vector $\mathbf{Q}=(0,0,\pi/c)$. Previously it has been shown that this interaction explains superconductivity in UPd_2Al_3 .⁵ We define the electron and magnetic exciton Green's functions as follows:

$$G_{\sigma\sigma'}(\mathbf{p}, i\omega_m) = -\left\langle T_\tau c_{\mathbf{p}\sigma}(\tau) c_{\mathbf{p}\sigma'}^\dagger(0) \right\rangle_{\text{FT}}, \quad D(\mathbf{q}, i\nu_n) = -\left\langle T_\tau a_{\mathbf{q}}(\tau) a_{-\mathbf{q}}^\dagger(0) \right\rangle_{\text{FT}}, \quad (2)$$

where $a_{\mathbf{q}}(\tau) = \alpha_{\mathbf{q}}(\tau) + \alpha_{-\mathbf{q}}^\dagger(\tau)$ and D is essentially the pseudospin susceptibility. The bare magnetic exciton Green's function is given by $D_0(\mathbf{q}, i\nu_n) = -\frac{\Delta_{\text{CEF}}}{2} \frac{1}{\nu_n^2 + \omega_{\mathbf{q}}^2}$. Due to the interaction of the magnetic excitons with conducting electrons, the feedback effect on the former results in

$$D = \frac{D_0}{1 - D_0 \Pi_0} = -\frac{2\omega_{\mathbf{q}}}{\omega^2 - \omega_{\mathbf{q}}^2 + 2\omega_{\mathbf{q}} \Pi_0}, \quad (3)$$

where the magnetic exciton self-energy is given by

$$\Pi_0(\mathbf{q}, i\omega_n) = g^2 \frac{\Delta_{\text{CEF}}}{\omega_{\mathbf{q}}} \chi_0(\mathbf{q}, i\omega_n). \quad (4)$$

Here, the spin susceptibility of the conduction electrons in the superconducting state is

$$\chi_0(\mathbf{q}, i\omega_n) = -\frac{1}{\beta} \sum_{i\omega_m, \mathbf{k}} [G(\mathbf{k}, i\omega_m) G^\dagger(\mathbf{k} + \mathbf{q}, i\omega_m + i\omega_n) + F(\mathbf{k}, i\omega_m) F^\dagger(\mathbf{k} + \mathbf{q}, i\omega_m + i\omega_n)], \quad (5)$$

where bare Green's functions of superconducting electrons are $G(\mathbf{k}, i\omega_m) = -\frac{i\omega_m + \xi_{\mathbf{k}}}{\omega_m^2 + \xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$, $F(\mathbf{k}, i\omega_m) = \frac{\Delta_{\mathbf{k}}}{\omega_m^2 + \xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. A straightforward evaluation of the sum over the Matsubara frequencies gives (at $T = 0$ K)

$$\text{Im } \chi_0(\mathbf{q}, \omega) = \frac{1}{4} \frac{1}{(2\pi)^3} \int d^3k \left(1 - \frac{\xi_{\mathbf{k}+\mathbf{q}} \xi_{\mathbf{k}} + \Delta_{\mathbf{k}} \Delta_{\mathbf{k}+\mathbf{q}}}{E_{\mathbf{k}+\mathbf{q}} E_{\mathbf{k}}} \right) \delta(\omega - E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}}). \quad (6)$$

The Fermi surface of the conducting electrons is almost like a cylinder with weak dispersion along the z direction. Neglecting the anisotropy of dispersion in the plane yields $\xi_{\mathbf{k}} = \epsilon_{k_\perp} + \epsilon_{k_z} - \mu = \epsilon_\perp w^2 + \epsilon_\parallel \cos(ck_z) - \mu$ ($\epsilon_\parallel \ll \epsilon_\perp$, $w = k_\perp/k_0 \leq 1$) and $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$. Here, we approximate the hexagonal unit cell by a circle with radius k_0 chosen so that the hexagon and the circle have the same area. Furthermore, we assume a parabolic dispersion in the plane. Due to the Ising-type anisotropy of the interaction between conduction electrons and magnetic excitons it has been previously found⁵ that both pure paramagnetic, *i.e.*, spin-singlet states $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

with $\cos(ck_z)$ momentum dependence and spin-triplet states ($S_z = 0$) $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ with $\sin(ck_z)$ have the highest (degenerate) superconducting transition temperature. Thus, in the following we will consider the two superconducting order parameters, $\Delta_{\mathbf{k}}^s = \Delta_0 \cos(ck_z)$ and $\Delta_{\mathbf{k}}^t = \Delta_0 \sin(ck_z)$ as the most relevant ones in this model.

Let us now discuss the consequences of the behavior of $\text{Im } \chi_0$ for the magnetic exciton dispersion which follows from Eq. (3). The dispersion of the magnetic exciton in the presence of coupling to the conduction electrons is

given by

$$\omega^2 = \omega_{\mathbf{q}}^2 - 2g^2\Delta_{\text{CEF}}\text{Re}\chi_0(\mathbf{q}, \omega) \quad (7)$$

In the normal paramagnetic state, $\text{Re}\chi_0$ is a constant at low frequencies determined in our case by the curvature of the Fermi surface along the k_z direction. At the same time $\text{Im}\chi_0 \propto -i\gamma\omega$, where γ is a Landau damping constant. Thus, the bare magnetic exciton acquires a linewidth and renormalizes slightly by a certain constant which changes the original position of $\omega_{\mathbf{q}}$ downwards. In the superconducting state the renormalization is strongly dependent on the gap symmetry. For example, in the conventional s -wave state $\text{Re}\chi_0$ is less than its normal state value. First, the s -wave superconducting gap gives a negative contribution to χ_0 as follows from the coherence factor in Eq. (6), and second it yields the spin excitation gap structure in $\text{Im}\chi_0$ as follows from the δ function. Therefore, the feedback of the conduction electrons on the magnetic exciton becomes weaker and yields a shift of the magnetic exciton dispersion towards higher frequencies in the superconducting state with respect to its normal state value.

At the same time, the unconventional character of the superconducting gap entails immediate consequences for Eqs. (6) and (7). Namely, at the Fermi surface (i.e., for $\xi_{\mathbf{k}} = 0$) one finds $\Delta_{\mathbf{k}+\mathbf{Q}}^s = -\Delta_{\mathbf{k}}^s$ as well as $\Delta_{\mathbf{k}+\mathbf{Q}}^{tr} = -\Delta_{\mathbf{k}}^{tr}$ where \mathbf{Q} is the antiferromagnetic wave vector. Thus, in both cases the anomalous coherence factor equals 2 for all k_z momenta which is in strong contrast to the usual s -wave symmetry of the superconducting gap. Simultaneously, the δ function in Eq. (6) starts to contribute for $\Omega_{cr}(k_z, q_z) = \text{Min}(E_{\mathbf{k}+\mathbf{z}q_z} + E_{\mathbf{k}}) = \sqrt{\epsilon_{\parallel}^2 [\cos(ck_z + cq_z) - \cos(ck_z)]^2 + (|\Delta_{k_z}| + |\Delta_{k_z+q_z}|)^2}$ which is determined by the value of the gap, $\Delta_{\mathbf{k}}$ and the quasiparticle dispersion along k_z axis, ϵ_{\parallel} . Note that $\Omega_{cr}^s(k_z, q_z = \pi/c) = 2|\cos(ck_z)|\sqrt{\Delta_0^2 + \epsilon_{\parallel}^2}$ and $\Omega_{cr}^{tr}(k_z, q_z = \pi/c) = 2\sqrt{\Delta_0^2 + (\epsilon_{\parallel}^2 - \Delta_0^2)\cos^2(ck_z)}$ for the singlet and triplet superconducting gap, respectively. It is interesting to note that for the singlet case there is no gap in $\text{Im}\chi_0$ and therefore, it is nearly the same as in the normal state⁶ [see Fig. 1(a)]. Then $\text{Re}\chi_0$ is a constant at low frequencies. Therefore the magnetic exciton dispersion will be simply shifted in proportion to the total value of $\text{Re}\chi_0$ exactly as in the normal state. Correspondingly, no strong feedback on the magnetic exciton due to superconductivity takes place.

However, one sees that in the case of the triplet order parameter $\text{Im}\chi_0$ will be gapped at least up to values of $\Omega_{cr}^{tr} = 2|\Delta_0|(\epsilon_{\parallel} \gg \Delta_0)$. Then due to a combined effect of the anomalous coherence factor and the δ function, a discontinuous jump in $\text{Im}\chi_0$ occurs at about $\omega = 2\Delta_0$ for the triplet order parameter. Via Kramers-Kronig transformation the discontinuous jump in $\text{Im}\chi_0$ yields a logarithmic singularity in $\text{Re}\chi_0$. Note, the logarithmic singularity in Fig. 1(b) is suppressed by a weak damping.

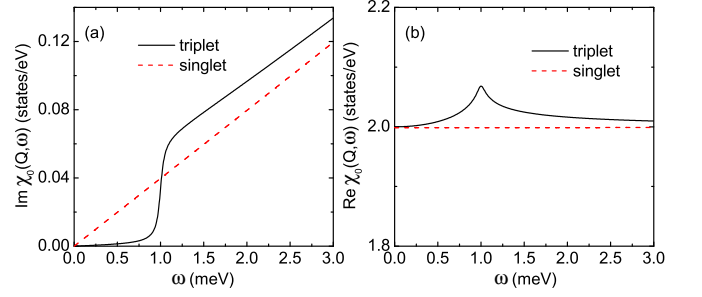


FIG. 1: (Color online) The (a) imaginary and (b) real parts of the longitudinal component of the conducting electrons spin susceptibility $\chi_0(\mathbf{Q}, \omega)$ as a function of frequency for singlet (red dashed curve) and triplet (black solid curve) Cooper pairing. The curves for the normal state (not shown) almost coincide with those for the spin singlet superconducting state. Here and in the following we use $T = 0.15$ K, $\Delta_0 = 0.5$ meV, $\epsilon_{\parallel} = 25$ meV and a damping parameter $35 \mu\text{eV}$ for the numerical calculations.

Furthermore, below Ω_{cr}^{tr} the $\text{Re}\chi_0$ is increased with respect to its normal state value for $\omega \neq 0$ as shown in Fig. 1(b).

A frequency dependence of the $\text{Re}\chi_0(\mathbf{Q}, \omega)$ can yield more than one solution of Eq. (7). In order to demonstrate how those solutions can be found above and below T_c we illustrate in Fig. 2 the possible characteristic behavior of $\omega_{\mathbf{q}}^2 - 2g^2\Delta_{\text{CEF}}\text{Re}\chi_0(\mathbf{q}, \omega)$. Here, we assume

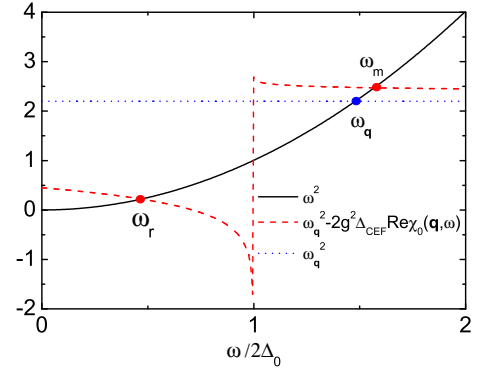


FIG. 2: (Color online) Illustration of the solutions of Eq. (7) at wave vector $\mathbf{q} = \mathbf{Q}$. In the normal state there is only one crossing point between the ω^2 curve (solid) with the $\omega_{\mathbf{q}}$ line (dotted) yielding the frequency of the magnetic exciton. Note that $\omega_{\mathbf{q}}$ may slightly differ from the bare exciton dispersion due to $\text{Re}\chi_0(\mathbf{Q}, \omega) = \text{const}$ in the normal state. In the superconducting state due to the strong frequency dependence of $\text{Re}\chi_0(\mathbf{q}, \omega)$ (and/or $\text{Re}\Pi_0$) one finds several intersecting points of ω^2 with $\omega_{\mathbf{q}}^2 - 2g^2\Delta_{\text{CEF}}\text{Re}\chi_0(\mathbf{q}, \omega)$. The lowest pole ($\omega_r < 2\Delta_0$) occurs at very small damping ($\text{Im}\chi_0$ is zero or small) resulting in a resonancelike peak in $\text{Im}D(\mathbf{q}, \omega)$. The second crossing point is not visible in $\text{Im}D$ due to a large peak in $\text{Im}\chi_0$ or strong damping around $2\Delta_0$. The third crossing point, ω_m occurs at energies larger than $2\Delta_0$ and represents the feedback effect of superconductivity on the magnetic exciton.

that in normal state the $\text{Re } \chi_0$ is almost frequency independent and magnetic exciton's peak position shifts slightly in superconducting state with respect to its normal state value. Due to the gap structure in superconducting state, depending on the value of g , a new pole may occur at energies less than $2\Delta_0$. If $\text{Im } \chi_0$ is small or zero at these frequencies, the total $\text{Im } D$, i.e., the spectral function of magnetic excitations, shows a resonance peak which occurs only in the superconducting state. This agrees well with experimental INS data³. Moreover, at higher energies one finds in addition two more poles in Eq. (7). The latter yields an additional structure in $\text{Im } D$ which is a renormalized magnetic exciton with finite damping. This typical behavior of the susceptibility can be found in Fig. 3.

So far we have ignored the coexistence of antiferromagnetism and superconductivity in UPd_2Al_3 for the conduction electrons.⁸ Antiferromagnetic order results in UPd_2Al_3 due to the interaction of neighboring uranium ions. This leads to a dispersion for exciton state and eventually to an antiferromagnetic instability and a new ground state.⁹ The unit cell is doubled and the Brillouine zone is correspondingly reduced. The new dispersion of the conducting electrons enters the expression for the spin susceptibility. Then the solutions of Eq. (7) must be redetermined. This is done in the following.

The total Hamiltonian is

$$H = H_0 + m \sum_{\mathbf{p}} \sigma c_{\mathbf{p}+\mathbf{Q}\sigma}^\dagger c_{\mathbf{p}\sigma} \quad (8)$$

$\text{Im } \chi_0(\mathbf{Q}, \omega) =$

$$\begin{aligned} & \sum_{\mathbf{k}} \frac{1}{8} \delta(\omega - 2E_{\mathbf{k}}^+) \left(1 - \frac{(\epsilon_{\mathbf{k}}^+)^2 - \Delta_{\mathbf{k}}^2}{(E_{\mathbf{k}}^+)^2} \right) \left(\frac{2m^2}{\epsilon_{k_z}^2 + m^2} \right) + \sum_{\mathbf{k}} \frac{1}{4} \delta(\omega - E_{\mathbf{k}}^+ - E_{\mathbf{k}}^-) \left(1 - \frac{\epsilon_{\mathbf{k}}^+ \epsilon_{\mathbf{k}}^- - \Delta_{\mathbf{k}}^2}{E_{\mathbf{k}}^+ E_{\mathbf{k}}^-} \right) \left(\frac{2\epsilon_{k_z}^2}{\epsilon_{k_z}^2 + m^2} \right) \\ & + \sum_{\mathbf{k}} \frac{1}{8} \delta(\omega - 2E_{\mathbf{k}}^-) \left(1 - \frac{(\epsilon_{\mathbf{k}}^-)^2 - \Delta_{\mathbf{k}}^2}{(E_{\mathbf{k}}^-)^2} \right) \left(\frac{2m^2}{\epsilon_{k_z}^2 + m^2} \right) . \end{aligned} \quad (9)$$

Here the first and the third terms describe the intraband quasiparticle pair creation while the second term refers to the corresponding interband process. Note that Eq. (9) contains two types of coherence factors, i.e., due to superconductivity and antiferromagnetic order, respectively. As usual, the low-energy behavior of $\text{Im } \chi_0$ is dominated by the intraband contributions. We also assume that the presence of antiferromagnetism does not change the qualitative behavior of the superconducting gap, i.e., the position of the line node and the corresponding change of sign of the superconducting order parameter remain the same although some higher harmonics may appear.¹¹ As in Eq. (6), the superconducting coherence factors equal 2 for k_z momenta close to the Fermi surface. At the same time, the reconstructed conduction bands in the AF state

where m denotes the value of the effective antiferromagnetic staggered field. This term leads to a splitting of the quasiparticle energy dispersion into two bands.¹¹ In particular, the Hamiltonian (8) can be easily diagonalized by a unitary transformation¹² and the resulting energy dispersions are $E_{\mathbf{k}}^\pm = \sqrt{(\epsilon_{\mathbf{k}}^\pm)^2 + \Delta_{\mathbf{k}}^2}$ with $\epsilon_{\mathbf{k}}^\pm = [\epsilon_{\mathbf{k}}^\pm \pm \sqrt{(\epsilon_{\mathbf{k}}^\pm)^2 + m^2}]$. Here, we have introduced $\epsilon_{\mathbf{k}}^+ = \frac{1}{2}(\xi_{\mathbf{k}} + \xi_{\mathbf{k}+\mathbf{Q}})$ and $\epsilon_{\mathbf{k}}^- = \frac{1}{2}(\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{Q}})$. The AF Fermi surface of the two bands $\epsilon_{\mathbf{k}}^\pm$ consists of two disjoint cylinders in the reduced AF BZ $|p_z| \leq \frac{\pi}{c}$ (see Ref. 10). In a pure AF state, the real part of the susceptibility χ_0 at low energies is determined by the intraband processes and can be approximated by $\chi_0(\mathbf{q}, \omega) \propto \sum_{\mathbf{k}} A_{\mathbf{k},q} \frac{f(\epsilon_{\mathbf{k}}^\pm) - f(\epsilon_{\mathbf{k}+\mathbf{q}}^\pm)}{\epsilon_{\mathbf{k}+\mathbf{q}}^\pm - \epsilon_{\mathbf{k}}^\pm + \omega}$ where $A_{\mathbf{k},q}$ is the AF coherence factor. At wave vector \mathbf{Q} for $\omega = 0$ the susceptibility is proportional to the density of states and decreases rapidly to zero as one increases frequency. This is a consequence of the equality $\epsilon_{\mathbf{k}}^\pm = \epsilon_{\mathbf{k}+\mathbf{Q}}^\pm$. Therefore the renormalization of the magnetic excitons due to conduction electrons can be safely ignored.

Most importantly, in the superconducting state coexisting with AF, the imaginary part of the spin susceptibility of the conduction electrons including intraband and interband scattering is given for $T=0$ K, $\mathbf{q} = \mathbf{Q}$, and $\omega > 0$ by

have only one-half the original period, i.e., $\epsilon_{\mathbf{k}}^\pm = \epsilon_{\mathbf{k}+\mathbf{Q}}^\pm$. Therefore all parts of the Fermi surface can be connected by the antiferromagnetic wave vector \mathbf{Q} and simultaneously have a sign change $\Delta_{\mathbf{k}+\mathbf{Q}} = -\Delta_{\mathbf{k}}$ of the gap except at the nodal points. As a result, $\text{Im } \chi_0(\mathbf{Q}, \omega)$ is non-zero for $\omega > 0$ due to the contribution of the nodal states both in the singlet and the triplet Cooper-pairing cases. With increasing frequency $\text{Im } \chi_0$ increases up to energies of about $2\Delta_0$ and then decreases [see Fig. 3(a)]. The functional dependence of $\text{Im } \chi_0$ at low frequencies resembles the behavior of the density of states except that the structure occurs at around $2\Delta_0$. Correspondingly, the real part of $\chi_0(\mathbf{Q}, \omega = 0)$ is the same as in a pure AF state. However, away from $\omega = 0$ it does not drop as in the pure AF state but increases quadratically up to about

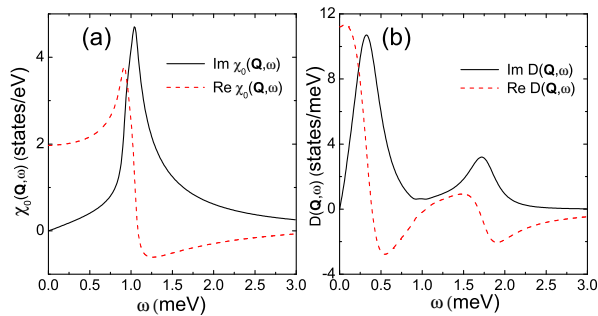


FIG. 3: (Color online) Results for $\chi_0(\mathbf{Q}, \omega)$ and $D(\mathbf{Q}, \omega)$ in the coexisting AF and singlet superconducting state. (a) Calculated real and imaginary parts of the longitudinal component of the conduction electron spin susceptibility, $\chi_0(\mathbf{Q}, \omega)$. (b) The real and imaginary part of the total pseudospin susceptibility $D(\mathbf{Q}, \omega)$. Here $m = 50$ meV, $g = 10$ meV. We use the gap function $\Delta_{\mathbf{k}} \propto \Delta_0 [\cos(ck_z) - \frac{1}{5} \cos(3ck_z) + \frac{1}{30} \cos(5ck_z)]$ (Ref. 7).

$2\Delta_0$ due to the structure of $\text{Im } \chi_0$ induced by the superconducting gap. Only then does $\text{Re } \chi_0$ drop to small values. Altogether $\text{Re } \chi_0(\mathbf{Q}, \omega)$ increases in the superconducting state for $\omega < 2\Delta_0$ due to the unconventional nature of the superconducting order parameter. However, the pure resonance (bound state) in $\text{Im } D$ is not realized due to finite damping. An additional pole in $\text{Im } D$ still exists at frequencies smaller than $2\Delta_0$ due to a strong increase of $\text{Re } \chi_0$ at small frequencies as shown in Fig. 3(b). At higher frequencies it becomes small and thus another pole appears corresponding to the broadened original magnetic exciton. Thus, $\text{Im } D$ has a two-pole structure as shown in Fig. 3(b). Note, in order to increase the intensity of the low-energy pole in $\text{Im } D$ we include the contribution of the higher harmonics to the gap function. As already mentioned, they are due to the presence of AF order¹¹.

Finally we discuss the dispersion of the magnetic excitations away from \mathbf{Q} along the q_z direction. In Fig. 4 we show the calculated momentum and frequency dependencies of $\text{Im } D(q_z, \omega)$. It is clear that as soon as $q_z \neq \pi/c$ the original magnetic exciton has a strong upward dispersion in the normal state. Therefore, effects connected with renormalization induced by superconductivity will also be shifted towards higher energies. The pole induced by superconductivity shows dispersion similar to the magnetic exciton [see Fig. 4]. For both singlet and triplet order parameters our results are in fair agreement with recent INS data.¹³ Namely, in the superconducting state one finds two distinct energy dispersions, one being the resonancelike feature with high intensity inside the superconducting gap and the second, that of localized magnetic excitons renormalized by the conducting electrons. Another interesting point worth noting is that due to the doubling of the unit cell and the equality $\varepsilon_{\mathbf{k}}^{\pm} = \varepsilon_{\mathbf{k}+\mathbf{Q}}^{\pm}$, the effect of the $\sin(ck_z)$ and $\cos(ck_z)$ gaps leads to a very similar behavior for $\text{Im } \chi_0$. The slight difference in

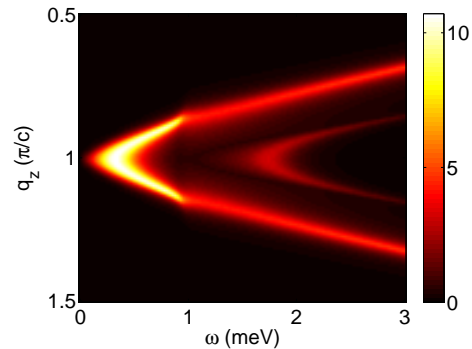


FIG. 4: (Color online) Contour plot of the imaginary part of the total pseudospin susceptibility as function of frequency, ω and q_z momentum. One clearly observes two distinct peaks at \mathbf{Q} . The one at low energies represents the resonance peak induced by the feedback of superconductivity and the one at higher ω is the renormalized magnetic exciton. Away from \mathbf{Q} both peaks disperse upward in energy following the behavior of the normal state magnetic exciton.

the absolute magnitude arises from the different densities of states at those regions of the Fermi surface where the maximum of the singlet and the triplet gaps occur. Altogether this does not change the functional form of $\text{Im } \chi_0$. We mention that thermal conductivity results in a rotating field¹⁴ are compatible with both $\cos(ck_z)$ and $\sin(ck_z)$ order parameters while the observed Knight shift¹⁵ seems to favor the former. Interestingly, we also found that a recently proposed superconducting gap with $\cos(2ck_z)$ symmetry¹⁶ does not lead to the formation of low-energy spin excitations around wave vector \mathbf{Q} in the superconducting gap. The reason is that its momentum dependence yields no change of the sign of the superconducting order parameter, $\Delta_{\mathbf{k}} = \Delta_{\mathbf{k}+\mathbf{Q}}$, and thus no constructive contribution can result from the anomalous coherence factor.

In conclusion, we have investigated the effects of superconductivity on the magnetic excitations in the unconventional superconductor UPd_2Al_3 . In particular, due to the change in sign of the superconducting order parameter the conduction electron susceptibility is enhanced in the superconducting state which yields an additional pole (bound state) in the total susceptibility. We further analyzed the role played by antiferromagnetism and found that its presence increases the spectral weight of the resonance due to the doubling of the unit cell. However, the resonance peak in the AF phase becomes a virtual bound state due to finite damping. Finally we point out that UPd_2Al_3 is another known example where the unconventional nature of the superconducting order parameter yields a structure in the magnetic susceptibility as in layered high- T_c cuprates. Therefore it can be regarded as a model system of unconventional superconductivity studied by inelastic neutron scattering.

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